

Quantum transport through a conducting bridge: Correlation between surface disorder and bulk disorder

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Abstract

We explore a novel transport phenomenon by studying the effect of surface disorder on electron transport through a finite size conductor with side coupled metallic electrodes. In the strong disorder regime the current amplitude increases with the increase of the surface disorder strength, while, the amplitude decreases in the weak disorder regime. This behavior is completely opposite to that of bulk disordered system. In this article we also investigate the effects of the size of the conductor and the transverse magnetic field on electron transport and see that the transport properties are significantly influenced by them.

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1 Introduction

A great challenge in the field of nanoscience and technology is to design and fabricate electronic devices on the nanometer scale with a specific geometry and composition. It is especially the field of molecular electronics that offers great potential where the electron transport is predominantly coherent [1, 2]. In 1974, Aviram *et al.* [3] first studied theoretically the electron transport through a molecule placed between two metallic contacts, and, later several experiments [4, 5, 6, 7, 8] have been carried out through different bridge systems. Electron transport through a conducting bridge is significantly influenced by several important factors like (a) structure of the conductor itself [9], (b) conductor-to-electrode coupling strength [10, 11, 12], (c) quantum interference effect [13, 14, 15, 16, 17, 18] and many other important parameters that are needed to describe the system. These effects have been described quite extensively in these references and there are also lot of papers in the literature where we have studied different aspects of the electron transport, but, the complete knowledge of the conduction mechanism through a bridge system is still unclear even today.

In the present paper we address a novel feature of electron transport considering the effect of surface disorder through a finite size conductor with side coupled electrodes. Advanced nanoscience and technology can easily fabricate a mesoscopic device in which charge carriers are scattered mainly by the surface boundaries and not by the impurities located in the inner core region [19, 20, 21]. The idea of such a system named as shell-doped nanowires has been given in a recent work by Zhong *et al.* [22] where the carrier mobility can be controlled nicely. The shell-doping confines the dopant atoms spatially within a few atomic layers in the shell region of nanowire. This is completely opposite to that of the conventional doping where the dopant atoms are distributed uniformly inside the nanowire. In this shell-doped nanowire system Zhong *et al.* [22] have obtained a peculiar behavior of electron transport in which the localization becomes weaker with the increase of the edge disorder strength in the strong disorder regime, while, the localization becomes stronger in the weak disorder regime. This reveals that the electron dynamics in a shell-doped nanowire undergoes a localization to quasi-delocalization transition as the disorder increases. Such enhancement of the electron diffusion length or in other words the increment of the car-

rier mobility in the strong disorder regime is due to the existence of quasi-mobility-edges in the energy spectrum of the system. This finding should provide significant applications in manipulation of carrier transport for shell-doped nanowires of single species and as well as for different types of co-axial heterostructured nanowires with modulation doping. A similar kind of novel quantum transport in the strong disorder regime has also been reported in a very recent work of Zhong *et al.* [23], where they have considered the order-disorder separated quantum films in which an anomalous transition is observed as the disorder strength increases. To reveal such an interesting phenomenon here we describe the electron transport through a small finite size conductor in which the impurities are located only in its surface boundary. From our study it is also observed that the electron transport through the conductor is significantly influenced by the size of the conductor which manifests the finite quantum size effects. In addition to these, here we also discuss the effect of transverse magnetic field on electron transport and get many interesting results. We utilize a simple tight-binding model to describe the system, and, adopt the Newns-Anderson chemisorption model [24, 25, 26] for the description of the electrodes and for the interaction of the electrodes to the conductor.

We organize the article as follows. In Section 2 we present the model and describe the method for the calculations. Section 3 illustrates the significant results, and finally, summary of the results will be available in Section 4.

2 Description of model and formalism

This section follows the description of the model and the methodology for the calculation of transmission probability (T), conductance (g) and current (I) through a finite size conductor attached to two semi-infinite one-dimensional (1D) metallic electrodes by using the Green's function formalism. The schematic view of such a bridge system is shown in Fig. 1, where the conductor is subjected to a transverse magnetic field B .

At sufficient low temperature and small applied voltage, the conductance g of the conductor is expressed through the Landauer conductance formula [27],

$$g = \frac{2e^2}{h}T \quad (1)$$

where the transmission probability T becomes [27],

$$T = \text{Tr} [\Gamma_S G_C^r \Gamma_D G_C^a] \quad (2)$$

In this expression G_C^r and G_C^a are the retarded and advanced Green's functions of the conductor, respectively. Γ_S and Γ_D describe the couplings of the conductor to the source and drain, respectively. The Green's function of the conductor is written in the form,

$$G_C = (E - H_C - \Sigma_S - \Sigma_D)^{-1} \quad (3)$$

where E is the energy of the source electron and H_C corresponds to the Hamiltonian of the conductor which can be expressed in the tight-binding representation within the non-interacting picture as,

$$H_C = \sum_i \epsilon_i c_i^\dagger c_i + \sum_{\langle ij \rangle} t (c_i^\dagger c_j e^{i\theta} + c_j^\dagger c_i e^{-i\theta}) \quad (4)$$

Here ϵ_i 's are the on-site energies and t corresponds to the nearest-neighbor hopping strength. Here we assume that the hopping strengths along the lon-

is the strength of disorder. Setting $\lambda = 0$ we get back the pure system with identical site potential W . Now to describe the two electrodes we use a similar kind of tight-binding Hamiltonian as prescribed in Eq.(4), where the on-site energy and the nearest-neighbor hopping strength are described by the parameters ϵ'_i and v , respectively. In Eq.(3), Σ_S and Σ_D represent the self-energies due to the coupling of the conductor to the source and drain, respectively, where all the information of the coupling are included into these two self-energies and are described through the use of Newns-Anderson chemisorption model [24, 25, 26]. In our tight-binding formulation the hopping strength of the conductor to the two metallic electrodes are represented by the parameters τ_S and τ_D , respectively. By utilizing the Newns-Anderson type model we can express the conductance in terms of the effective conductor properties multiplied by the effective state densities involving the coupling. This permits us to study directly the conductance as a function of the properties of the electronic structure of the conductor within the electrodes.

The current passing across the conductor can be assumed as a single electron scattering process between the two reservoirs of charge carriers. The current-voltage (I - V) characteristics can be computed through the expression [27],

$$I(V) = \frac{e}{\pi\hbar} \int_{-\infty}^{\infty} (f_S - f_D) T(E) dE \quad (5)$$

where $f_{S(D)} = f(E - \mu_{S(D)})$ gives the Fermi distribution function with the electrochemical potential $\mu_{S(D)} = E_F \pm eV/2$. For the sake of simplicity, here we assume that the entire voltage is dropped across the conductor-to-electrode interfaces and this assumption does not significantly affect the qualitative aspects of the current-voltage characteristics. Such an assumption is based on the fact that the electric field inside the conductor, especially for short conductors, seems to have a minimal effect on the g - E characteristics. On the other hand, for bigger conductors and higher bias voltage, the electric field inside the conductor may play a more significant role depending on the size and the structure of the conductor [28], yet the effect is much small.

Throughout the paper we describe our results at very low temperature (4 K), but the qualitative features of all the results are invariant up to some finite temperature (~ 300 K). For simplicity we take the units $c = e = \hbar = 1$ in our present discussion.

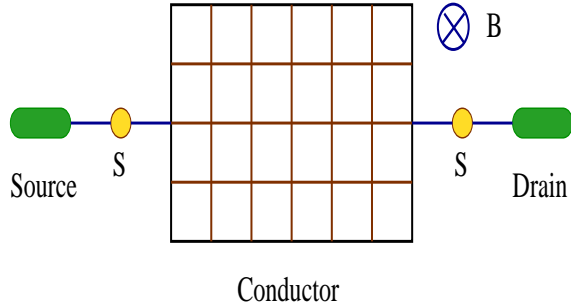


Figure 1: (Color online). A finite size conductor attached to two 1D semi-infinite metallic electrodes through lattice sites S and S . To get a surface disordered conductor, the impurities are introduced only in the boundary surface which is described by the black color. While, for the bulk disordered case, the impurities are given in the surface as well as in the core regions.

gitudinal and the transverse directions are identical to each other, for simplicity. The phase factor $\theta = (2\pi/\phi_0) \int_0^a \vec{A} \cdot d\vec{l}$, where a is the lattice spacing and $\vec{A}(By, 0, 0)$ is the vector potential associated with the magnetic field B . In order to introduce the impurities in the conductor we set the site energies (ϵ_i 's) in the form of incommensurate potentials through the expression $\epsilon_i = \sum_i W \cos(i\lambda\pi)$ where λ is an irrational number, and as a typical example, we take it as the golden mean $(1 + \sqrt{5})/2$. W

3 Results and discussion

Here we focus our results and discuss the correlation effect between the surface disorder and bulk disorder on electron transport through a finite size conductor with side coupled metallic electrodes. The effects of the transverse magnetic field and the size of the conductor are also described in the subsequent parts. Our results suggest the principles for understanding and control of the electron transport through any bridge system. Here we use the parameters N_x and N_y to denote the total number of atomic sites of the conductor along the x and y directions, respectively. We choose N_y as odd always and connect the electrodes symmetrically to the conductor as presented in Fig. 1. Throughout our study we set the values of the different parameters as follows: the hopping strengths of the conductor

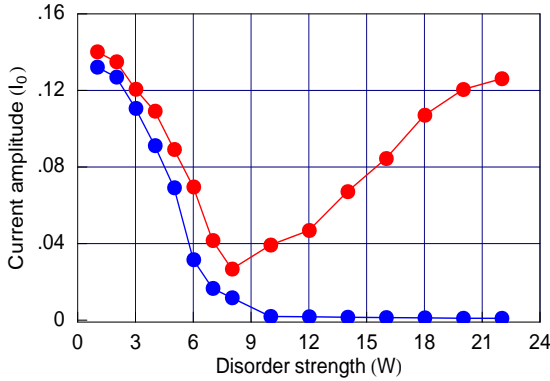


Figure 2: (Color online). Typical current amplitude I_0 as a function of the disorder strength W for the conductor with $N_x = 6$ and $N_y = 5$, in the absence of any magnetic field i.e., $B = 0$. The red and blue curves correspond to the results for the surface and bulk disordered conductors, respectively.

to the electrodes (source and drain) $\tau_S = \tau_D = 0.5$ and the nearest-neighbor hopping integral $t = 3$. In the electrodes, we fix the hopping strength v between the nearest-neighbor sites at 3 and the on-site energies (ϵ_i 's) of all the atomic sites in these electrodes are taken as zero. The Fermi energy E_F is set to 0.

In Fig. 2 we plot the typical current amplitudes I_0 as a function of the disorder strength W for a finite size conductor considering $N_x = 6$ and $N_y = 5$. The transverse magnetic field B is set at 0 and the typical current amplitudes are computed at the applied bias voltage $V = 1$. The red and blue curves correspond to the results for the surface and bulk disordered conductors, respectively. Here we introduce

only the diagonal disorder considering the on-site energies from the incommensurate potential distribution function as stated earlier, and in the obvious reason we do not take any disorder averaging. For the bulk disordered conductor, the current amplitude gradually decreases with the increase of the impurity strength W . This behavior can be clearly understood from the theory of Anderson localization where we get more localization with higher dis-

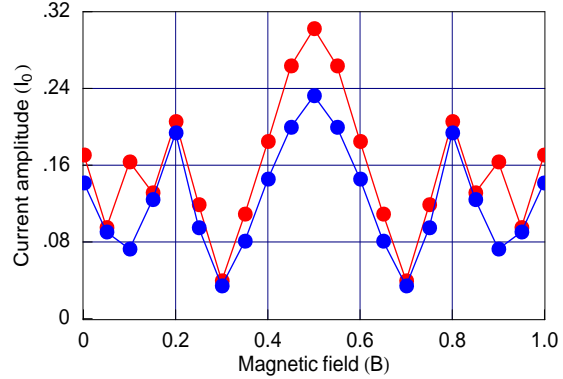


Figure 3: (Color online). Typical current amplitude I_0 as a function of the magnetic field B for a conductor with $N_x = 6$ and $N_y = 5$ in the weak disorder ($W = 3$) regime. The red and blue curves correspond to the results for the surface and bulk disordered cases, respectively.

order strength and this is a well known feature in the study of electron transport. A dramatic feature is observed for the conductor when the impurities are introduced only in its surface boundary. The current amplitude decreases initially with the increase of the impurity strength and after reaching a minimum it again increases with the strength of the impurity. This is completely opposite in nature from the bulk disordered case, where current amplitude always decreases with the impurity strength. Such an anomalous behavior for the surface disordered case can be explained in the following way. We can treat the surface disordered conductor as a coupled system where the disordered surface is coupled to the inner core perfect region, according to the description given by Zhong *et al.* [22]. Thus we can predict that, in the absence of any coupling, the localized states are obtained at the surface region, while we get the extended states in the inner core perfect region. For the coupled system, the coupling between these localized states to the inner core extended states is strongly influenced by the strength of surface disorder. In the limit of

weak disorder the coupling is strong, while the coupling effect becomes less important in the limit of strong disorder. Therefore, in the weak disorder regime the electron transport is strongly influenced by the impurities at the surface in which the electron states are scattered more, and accordingly, the current amplitude decreases. On the other hand, for the stronger disorder regime the inner core extended states are less influenced by the surface disorder and the coupling effect gradually decreases with the im-

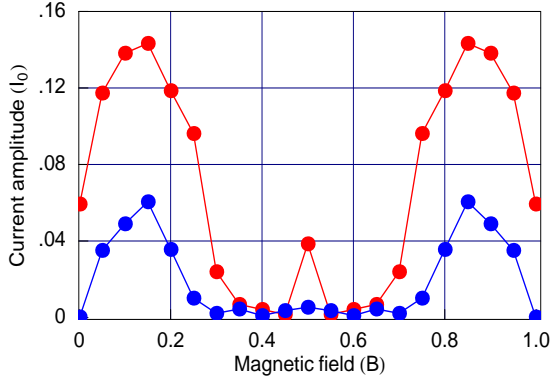


Figure 4: (Color online). Typical current amplitude I_0 as a function of the magnetic field B for a conductor with $N_x = 6$ and $N_y = 5$ in the strong disorder ($W = 15$) regime. The red and blue curves correspond to the identical meaning as in Fig. 3.

purity strength. Therefore, the current amplitude increases gradually in the strong disordered regime. For the large enough impurity strength, the inner core extended states are almost unaffected by the impurities at the surface and in that situation we get the current only due to the inner core extended states which is the trivial limit. So the exciting limit is the intermediate limit of W .

To investigate the effect of the transverse magnetic field on electron transport now we describe the results those are plotted in Figs. 3 and 4. Here we take the same system size as considered in Fig. 2. The red and blue curves correspond to the surface and bulk disordered conductors, respectively, where Fig. 3 represents the behavior of the current amplitudes in the weak disorder ($W = 3$) regime and the results for the limit of strong disorder ($W = 15$) are shown in Fig. 4. The typical current amplitudes are calculated at the same bias voltage as mentioned earlier. Both for the two limiting cases of the disorder strength, the current amplitude varies periodically with the magnetic field B , showing ϕ_0 ($= ch/e$, the elementary flux-quantum) periodicity.

In the limit of weak disorder, the current amplitudes both for the surface and bulk disordered conductors are comparable to each other in the whole range of B showing a maximum around $B = 0.5$ (Fig. 3). On the other hand, for the case of strong disorder, the current amplitudes are comparable only in the small range around $B = 0.5$ (Fig. 4), while for all other ranges the current amplitude in the surface disordered conductor is very large than that of the bulk disordered case which indicates that in these ranges the inner core extended states are much less affected by the surface disorder. All these results are also valid for the conductors with other system

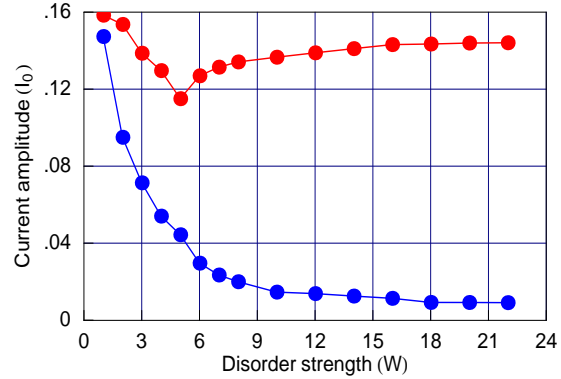


Figure 5: (Color online). Typical current amplitude I_0 as a function of the disorder strength W for a conductor with $N_x = 7$ and $N_y = 5$, in the absence of any magnetic field. The red and blue curves represent the identical meaning as in Fig. 2.

sizes (N_x and N_y). Thus we can predict that in the limit of strong disorder the correlation among the surface disorder and bulk disorder strongly depends on the strength of the transverse magnetic field B .

To emphasize the finite quantum size effects on electron transport, in Fig. 5 we plot the results for the bridge system considering $N_x = 7$ and $N_y = 5$. The results are plotted for $B = 0$ those are computed at the typical bias voltage $V = 1$ and the red and blue curves represent the identical meaning as in Fig. 2. In the two disordered regimes the characteristic features of the current amplitudes both for the surface and bulk disordered conductors are similar to that as given in Fig. 2. But the significant observation is that the overall current amplitude for this surface disordered conductor is much larger than that of the results as observed for the surface disordered conductor with $N_x = 6$ and $N_y = 5$ (see the red curve of Fig. 2). This behavior can be explained as follows. For a fixed N_y ($N_y = 5$) as we

increase the system size from $N_x = 6$ to $N_x = 7$, the ratio of the surface to inner core region decreases (1.5 to 1.33), and accordingly, the surface effect becomes less important. Therefore, the current carried by the inner core region will be less affected by the surface disorder which provides greater current amplitude. Now, if we change the system size in such a way that the ratio of the surface to inner core region increases, then we will get lesser current in the overall region. Another important observation is that, the typical current amplitude where it goes to a minimum strongly depends on the system size which is clearly visible from the red curves plotted in Figs. 2 and 5. These results reveal the finite quantum size effects in the study of electron transport phenomena.

4 Concluding remarks

To summarize, we have studied a peculiar effect of the surface disorder on quantum transport through a finite size conductor with side coupled electrodes by using the Green's function technique, based on the tight-binding formulation. For a surface disordered conductor our results have provided an anomalous behavior in which the current amplitude increases with the increase of the disorder strength in the strong disorder regime, while the current amplitudes decreases in the weak disorder regime. This feature is completely opposite to that of the bulk disordered conductor in which the current amplitude decays gradually with the increase of the impurity strength. The model studied here is a generalization of the novel class of quantum structures named as shell-doped nanowires [22], order-disorder separated quantum films [23], where the anomalous transition is observed in the strong disorder regime. From our study of the electron transport in the presence of transverse magnetic field we have observed that, in the limit of strong disorder the correlation among the surface disorder and bulk disorder strongly depends on the strength of the magnetic field. Finally, to emphasize the finite quantum size effects we have studied the electron transport by varying the system size and the results have predicted that the typical current amplitude where it goes to a minimum significantly depends on the size of the conductor.

Throughout our study we have considered several important assumptions by neglecting the effects of all the inelastic scattering processes, the electron-electron correlation, the Schottky effect, the static Stark effect, etc. More studies are expected to take

into account all these assumptions for our future study.

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